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Materials by Design - Computational Alloy Design for Corrosion




Charlie Kuehmann

QUESTEK®
INNOVATIONS LLC
Materials By Design®
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Report Documentation Page

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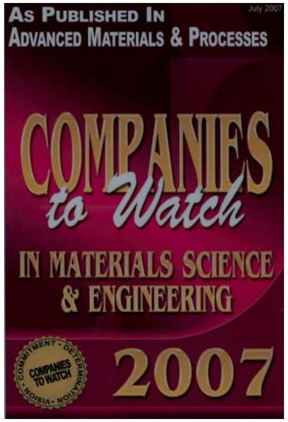
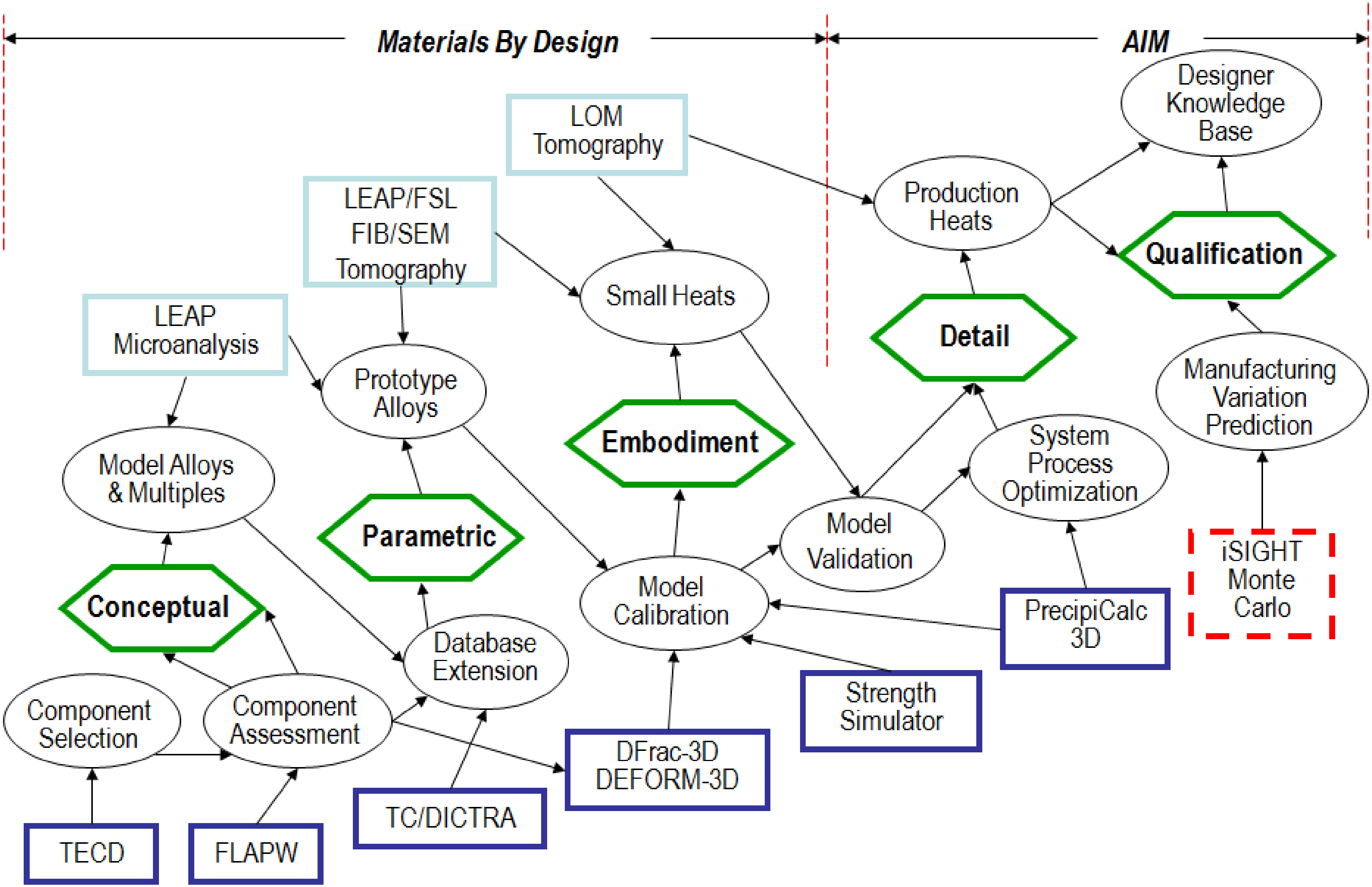
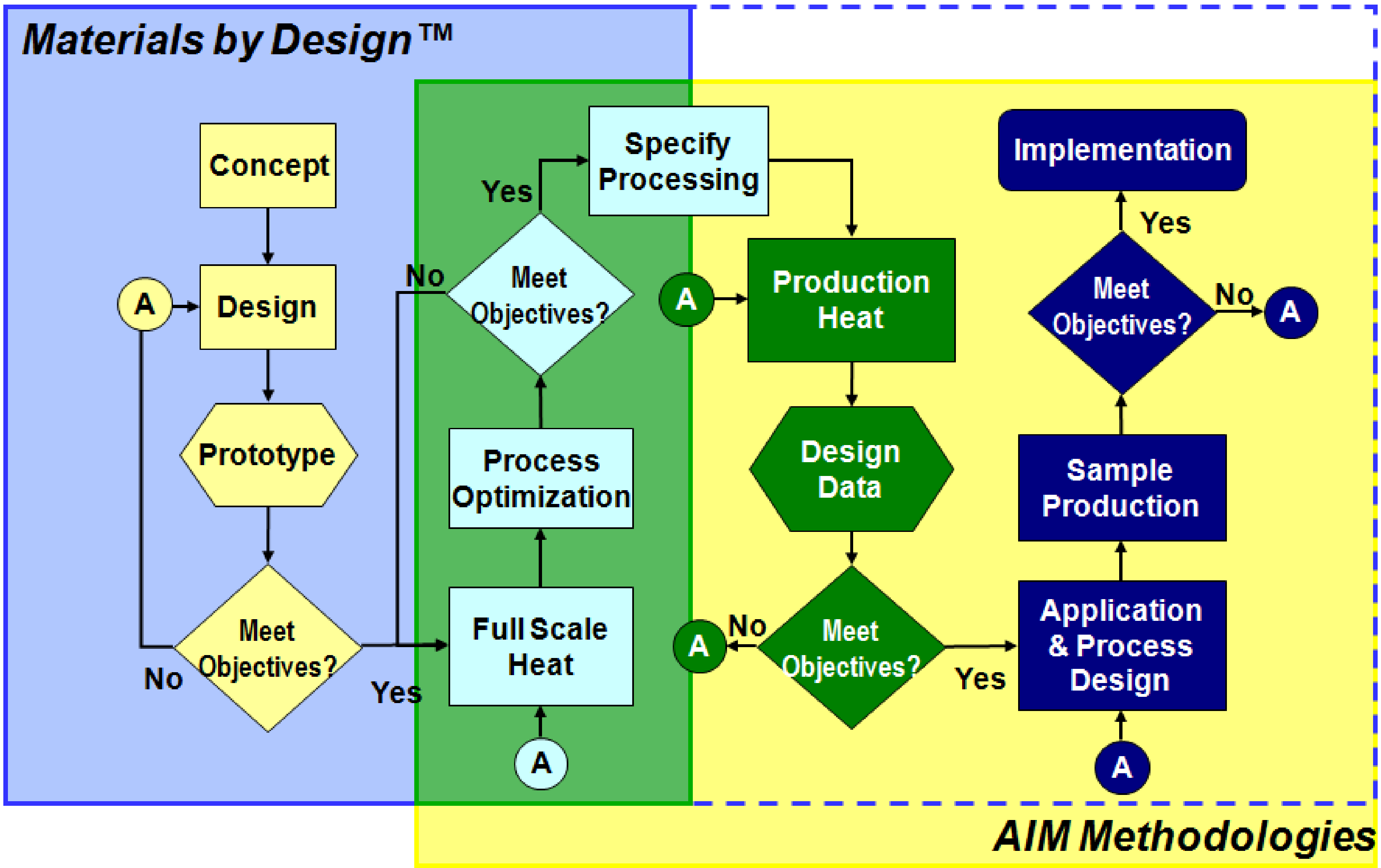
Background - QuesTek Innovations LLC

- 16 engineers, 9 with PhDs; founded 1997
- Rapidly designing, developing, qualifying and inserting new materials using computational methods on integrated basis
- Creates IP; licenses to OEMs or alloy producers/processors
- 4 alloys licensed: *Ferrium*® M54™, C61™, C64™ and S53®
- Working with many colleagues in industry and academia
- ~10 major new alloys in development
- 30+ patents awarded or pending worldwide
- Serving industry and government
- Recipient of many business and technology awards
- Expanding our staff

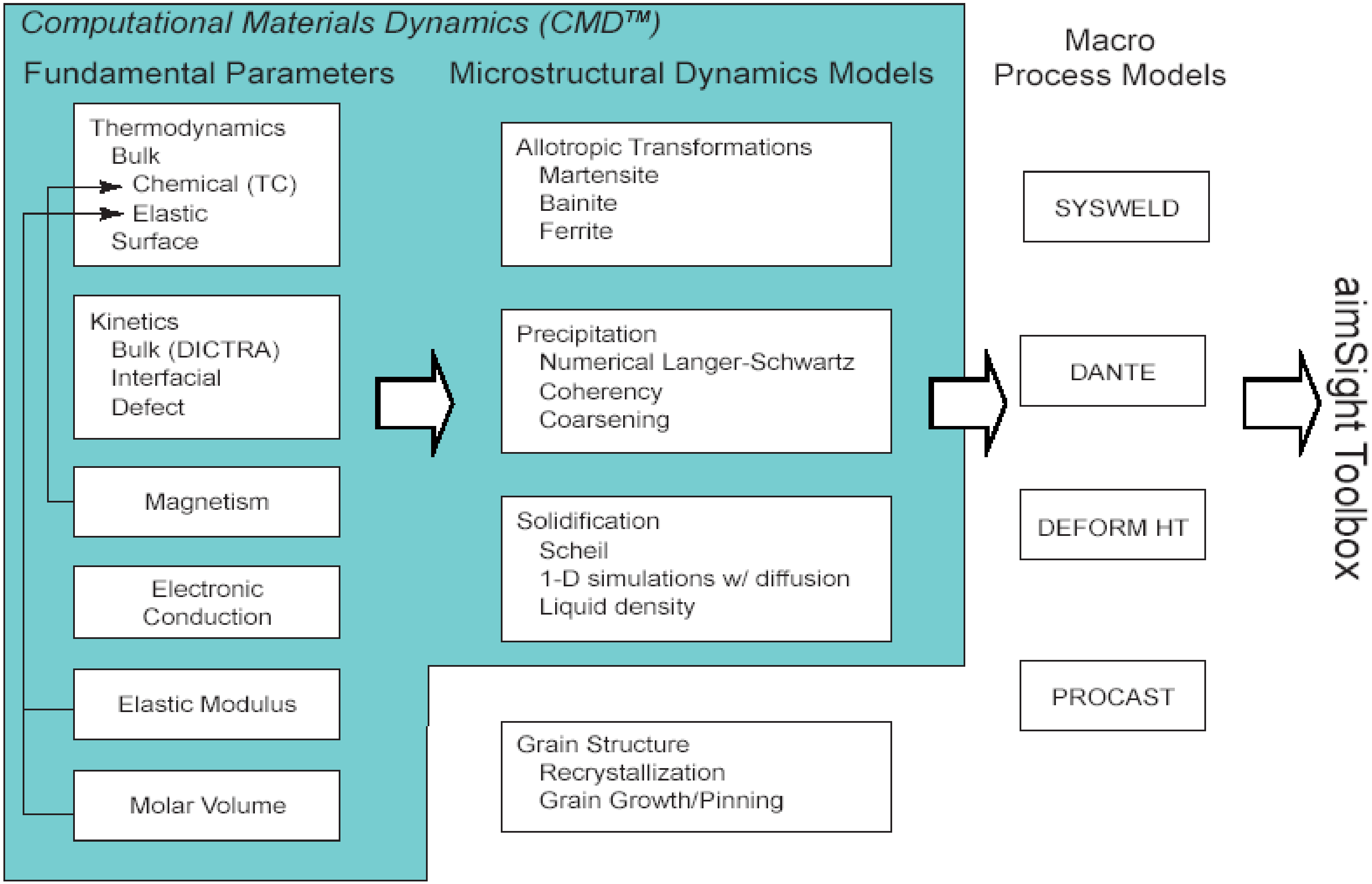



Materials By Design
AIM
LOM Tomography
Designer Knowledge Base
LEAP/FSL FIB/SEM Tomography
Production Heats
Qualification
Small Heats
LEAP Microanalysis
Detail
Prototype Alloys
Embodiment
Manufacturing Variation Prediction
Model Alloys & Multiples
System Process Optimization
Parametric
Model Validation
Conceptual
Model Calibration
iSIGHT Monte Carlo
Database Extension
PrecipiCalc 3D
Component Selection
Component Assessment
Strength Simulator
DFrac-3D DEFORM-3D
TC/DICTRA
TECD
FLAPW

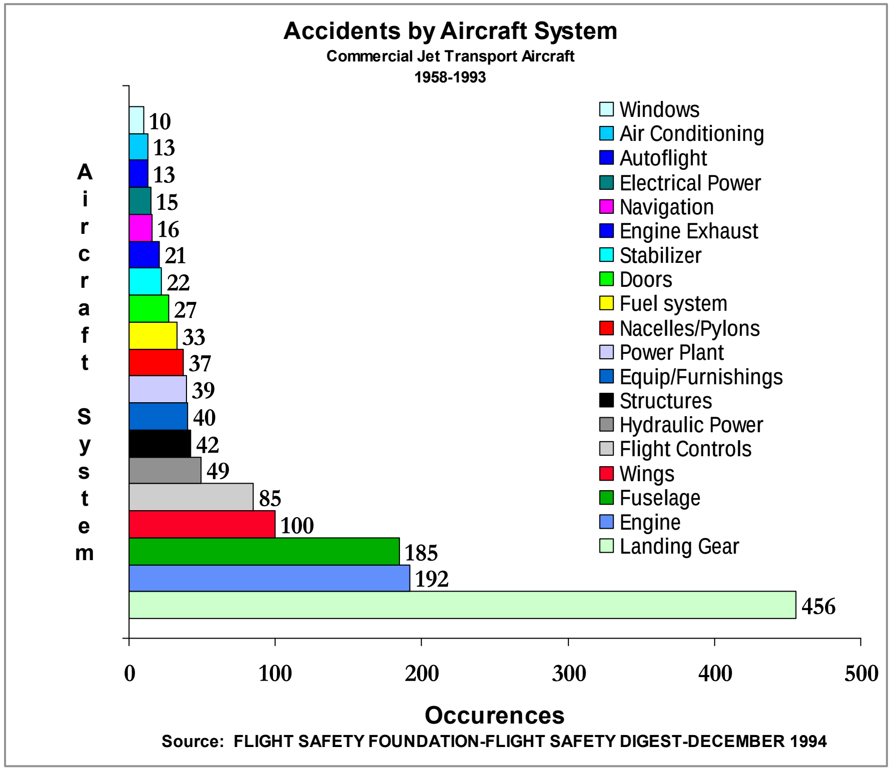
Accelerating the Materials Development Cycle



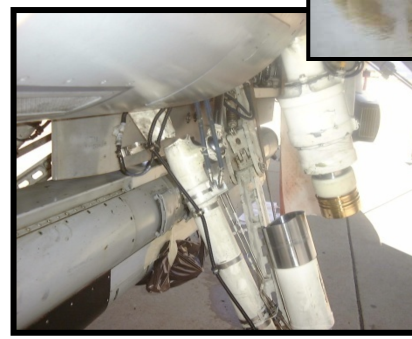
Process-Structure Modeling



A First Example of Materials Design for Corrosion



SCC failures



HE failures

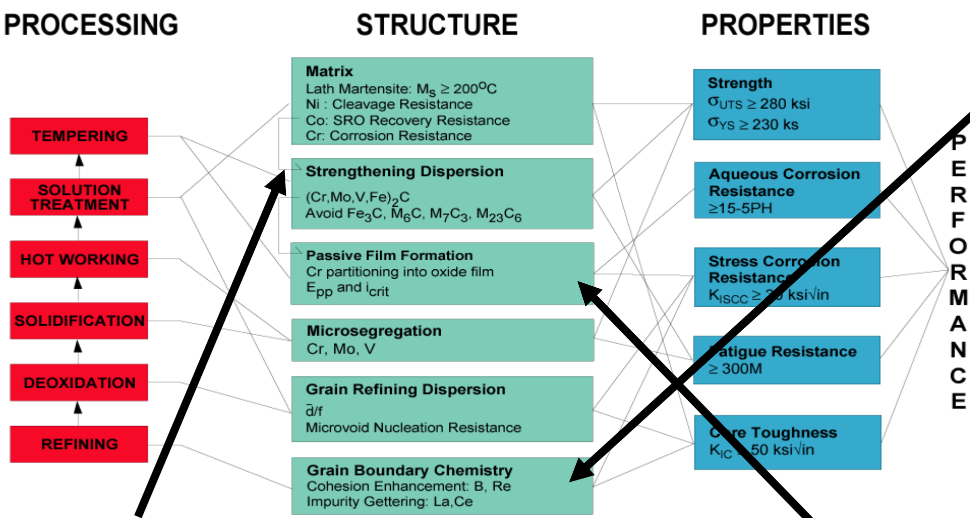
Issues:

Over $200 million spent in LG per year
80% corrosion related
SCC failures
Cad plating used to protect current steel
known carcinogen (Hill AFB ~ 2000 lbs/yr)

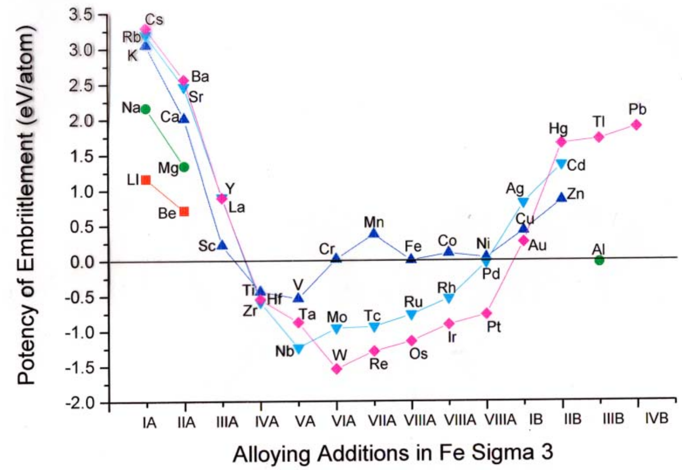
Benefits:

Dramatic reduction in LG cost (60%)
savings of $120 million per year
Significant reduction in SCC failures
Cadmium plating not required
General corrosion mitigated
80% of Steel Condemnations Avoided

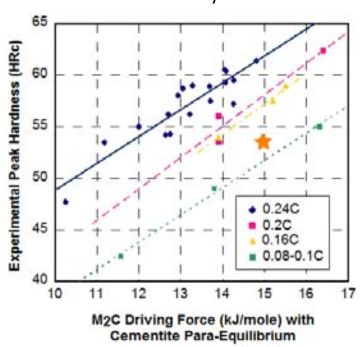
Design Models Founded on Scientific Understanding but Implemented for Optimization

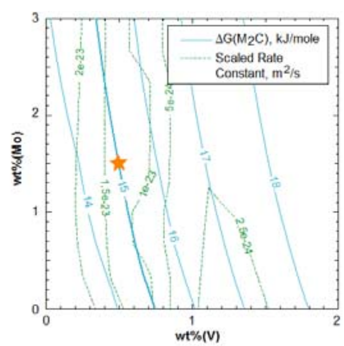


Chris Kantner - "Quantum Steel"
PhD thesis Northwestern, 2001

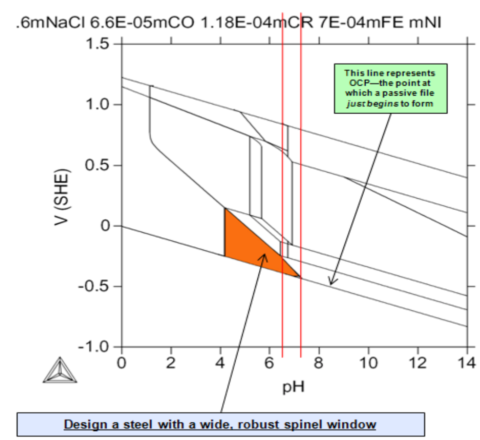


Charlie Kuehmann - "Thermal Processing Optimization of Nickel-Cobalt Ultra High-Strength Steels"
PhD thesis Northwestern, 1994





Carelyn Campbell - "Systems Design of Stainless Bearing Steel"
PhD thesis Northwestern, 1996



Corrosion modeling

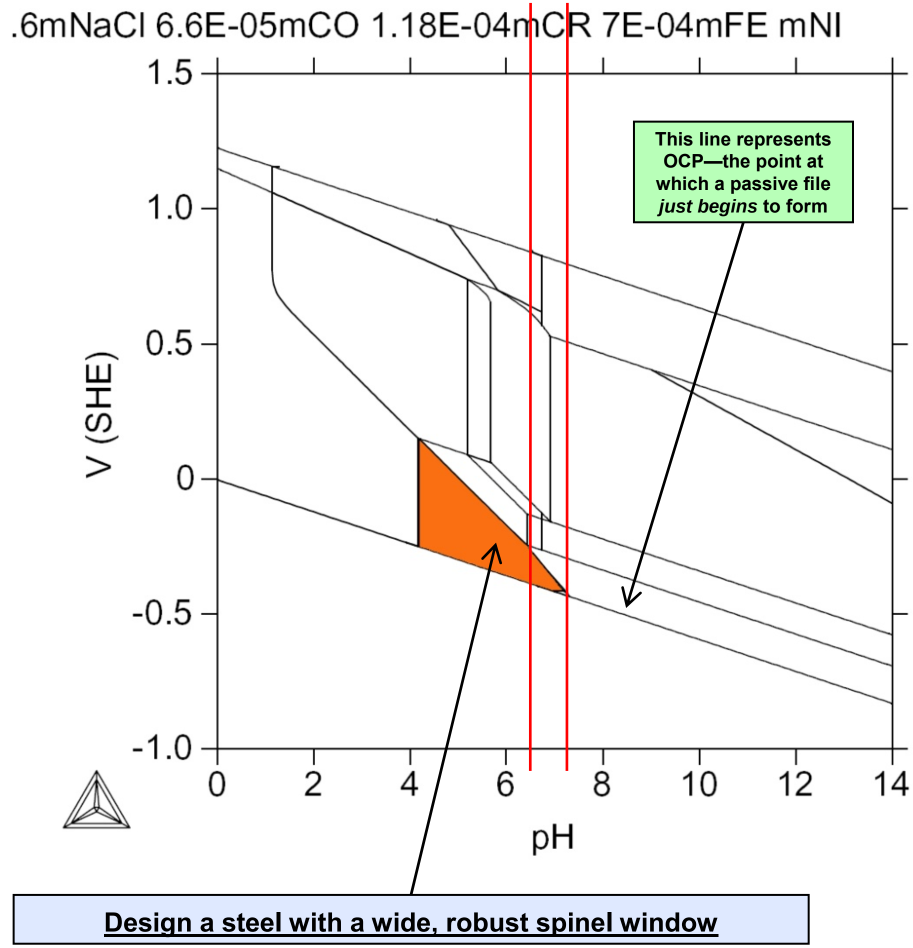
Pourbaix diagrams

Design a steel with a wide, robust spinel window

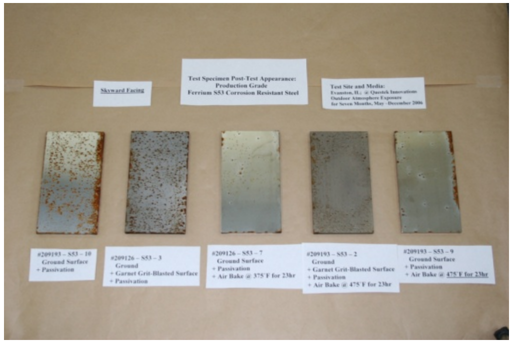
ASTM B117 pH ≈ 6.5-7.2

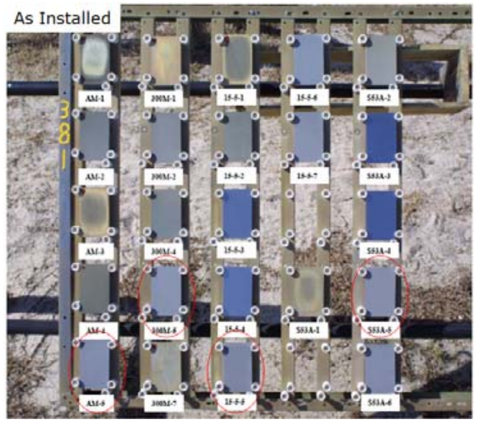
Diagrams not very sensitive to composition
- **Revised oxide TDB**

On the "oxide formation" side of things
- **Equilibrium**



S53 Corrosion Behavior

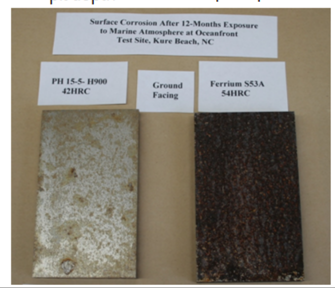




Initial Studies: 12 months

PH 15-5 (195 ksi) ~ 0.0005" pit depth

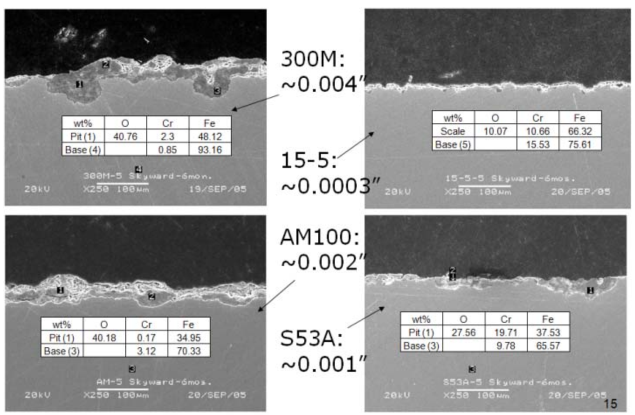
S53A (285 ksi) 0.001" ~ 0.002" pit depth



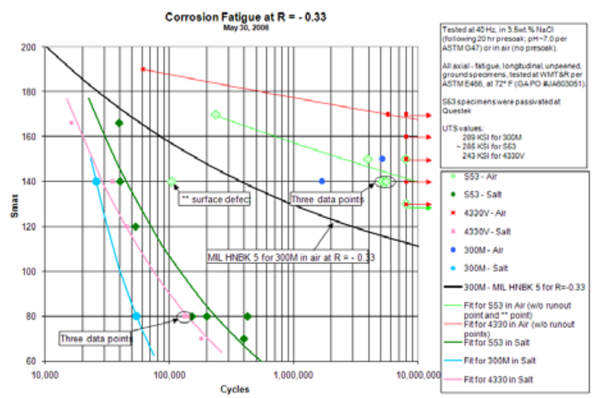
Follow-up Studies: 3 months

S53 (AMS 5922) (288 ksi) 0.001" ~ 0.002" pit depth

Exposure tests at QuesTek (left) and Kure beach (center, right)

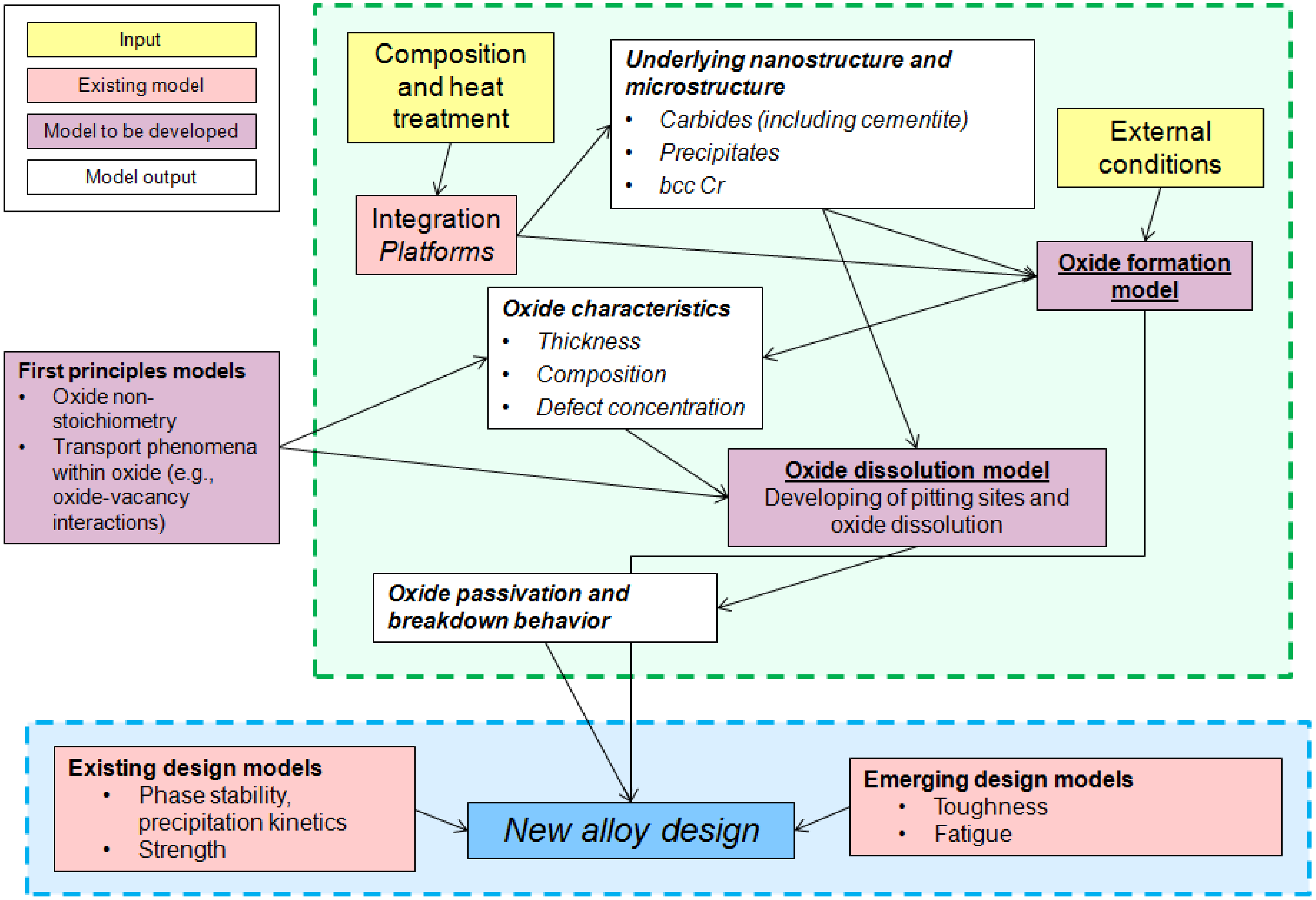


Characterization of corrosion pits

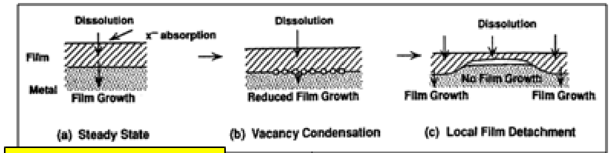


Corrosion fatigue testing

A Corrosion Modeling Architecture



Multiscale representation of the metal/oxide system



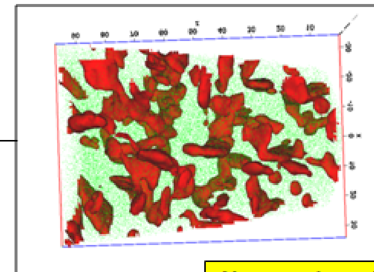
Oxide dissolution

Oxide

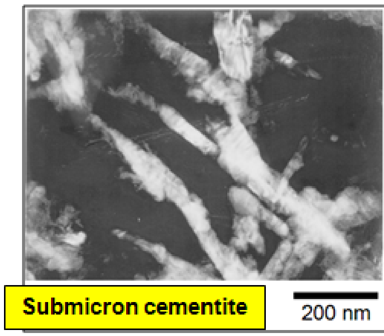
- *Oxide layer*
  - *Formation*
  - *Development of pitting sites and dissolution*

- *Underlying microstructure and nanostructure*
  - *Solidification microstructure*
  - *Inclusions (sulfides, oxides, etc.)*
  - *Austenite (retained, precipitated, etc.)*
  - *Martensitic lath structure*
  - *Carbides*
    - *Nanoscale*
    - *Cementite*
  - *Other strengthening precipitates*
  - *Nanoscale bcc Cr*

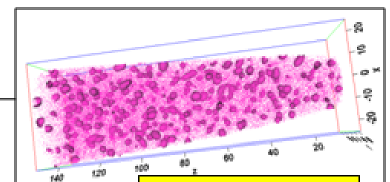
Base metal



Nanoscale carbides



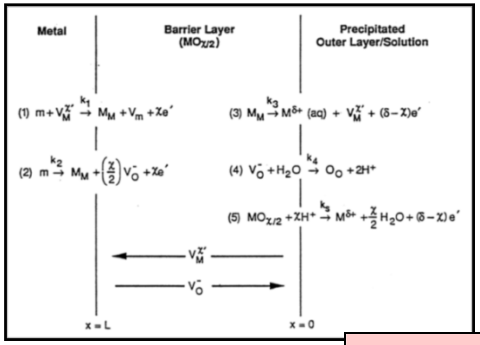
Submicron cementite



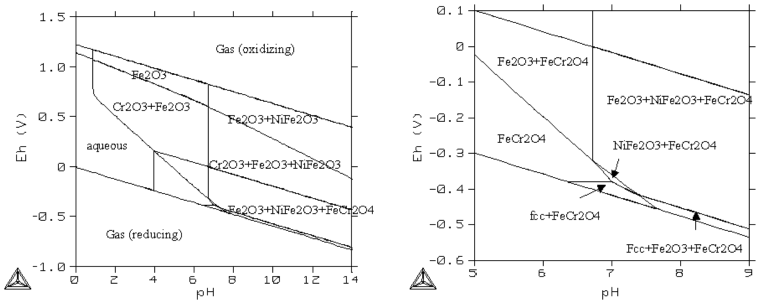
Nanoscale bcc Cr

Oxide formation and dissolution

Oxide formation (PDM framework, left;)

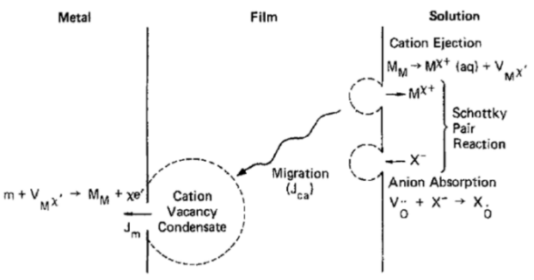


Oxide formation

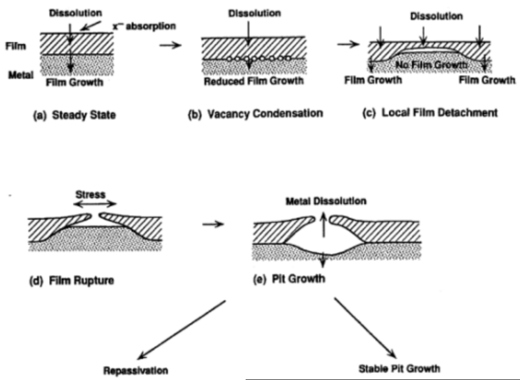


Calculated Pourbaix diagrams

Oxide dissolution (PDM framework)



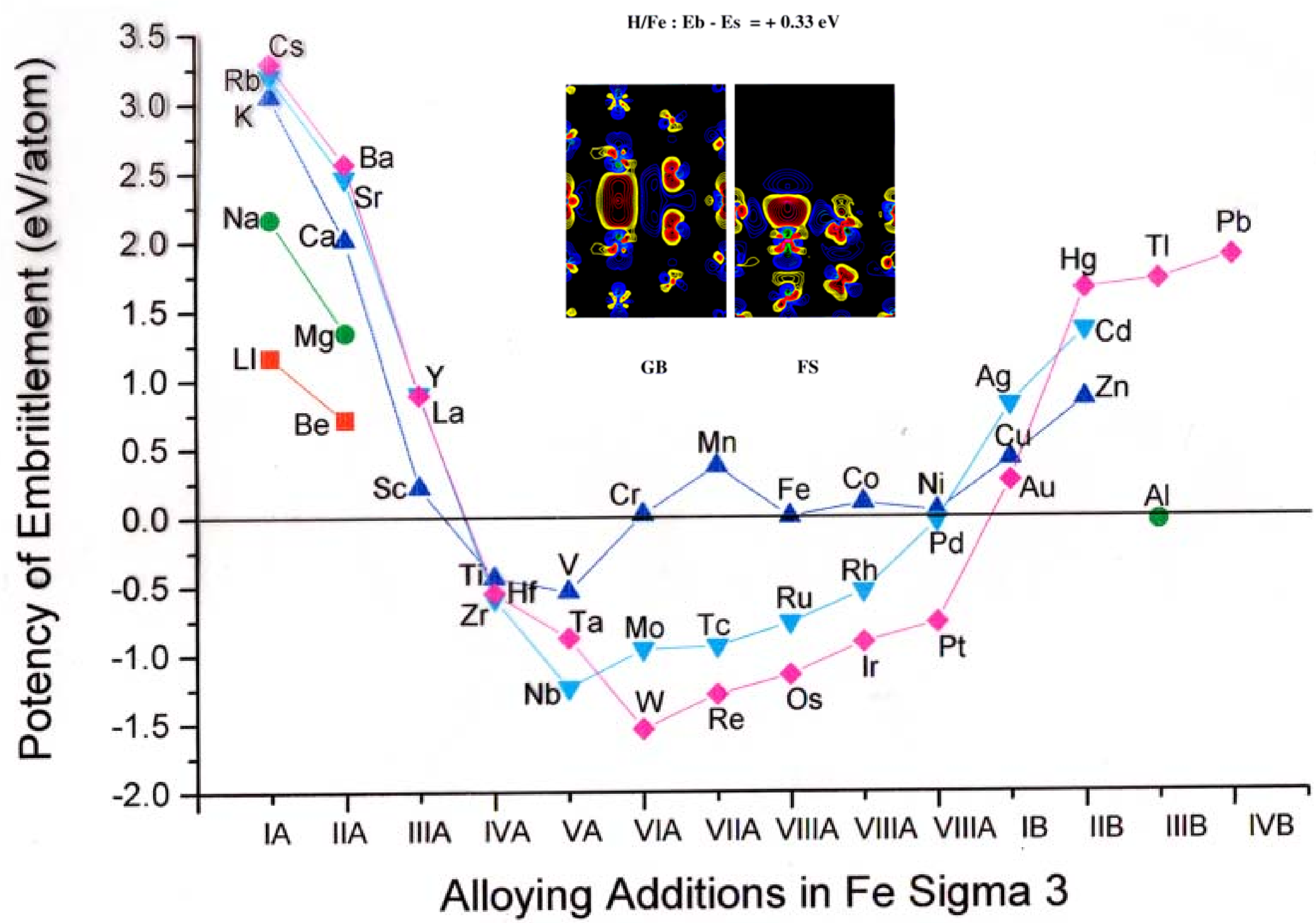
Cation condensation



Oxide dissolution and rupture

Figures from D.D. Macdonald, *Pure and Applied Chemistry*, 71(6), 1999

Quantum Mechanics Insights into SCC resistance



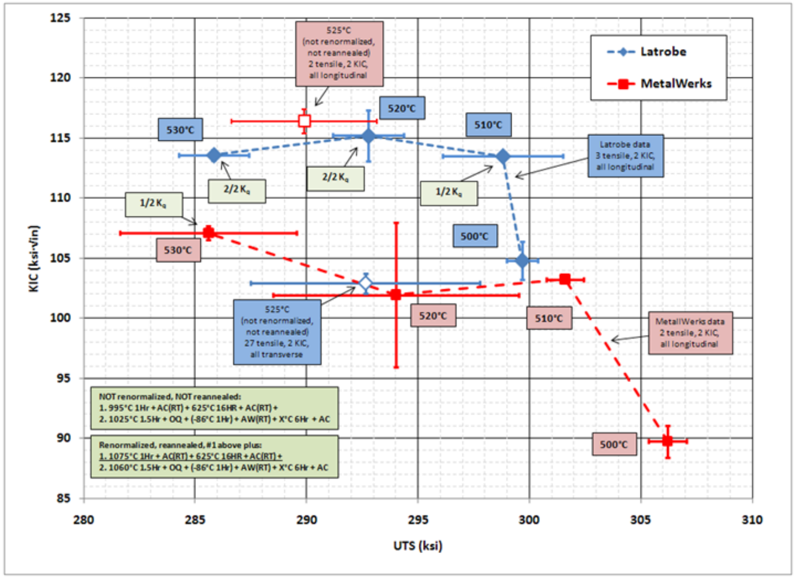
Example: Lower Cost Designs for Optimal SCC Resistance

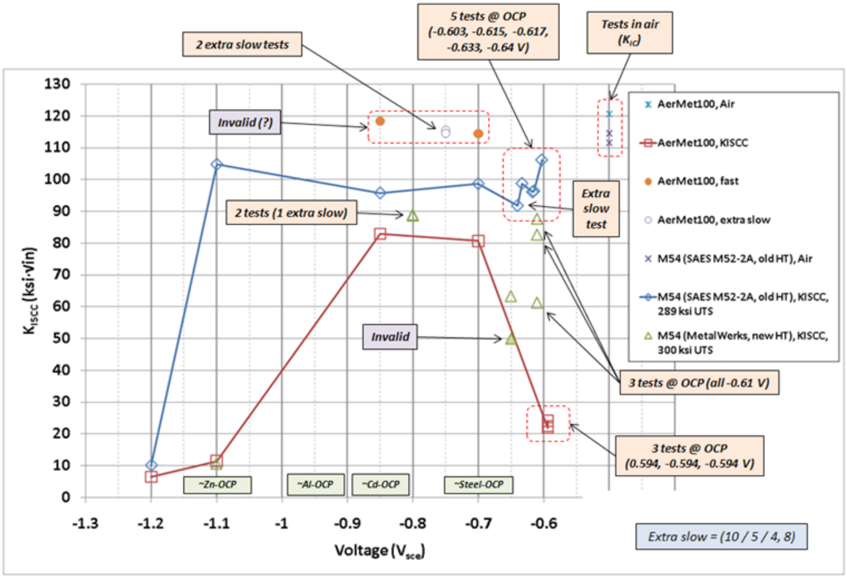
- *Ferrium* M54
  - Navy SBIR program
    - Navy SBIR topic N07-032, “Computational Design of Advanced Alloys for USN Landing Gear.” Currently in Phase II (contract N68335-08-C-0288). TPOCs Amy Little and Michael Leap.
  - Phase I: 2007-2008
  - Phase II Base: 2008-2010
  - Full-scale production, demonstration of 1% minimum properties, patented composition with commercial licensee





LATROBE SPECIALTY STEEL COMPANY





Schematic of an electrochemical framework

Input

Existing model

Model developed in program

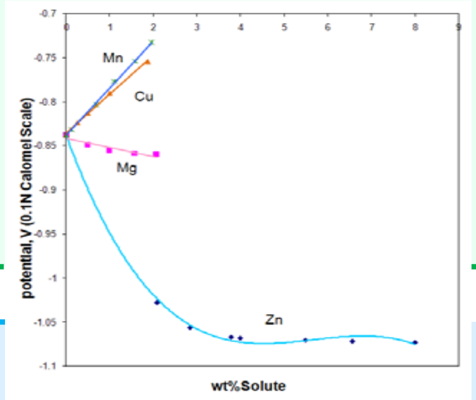
Model output

Composition and heat treatment

QuesTek's *CMD*

Underlying nanostructure and microstructure
- ***FCC matrix***
- ***Strengthening precipitates***
- ***Dispersoids***
- ***Constituents***

a. Corrosion Potential of matrix (composition dependant)
b. Corrosion potential of intermetallics (composition dependant)

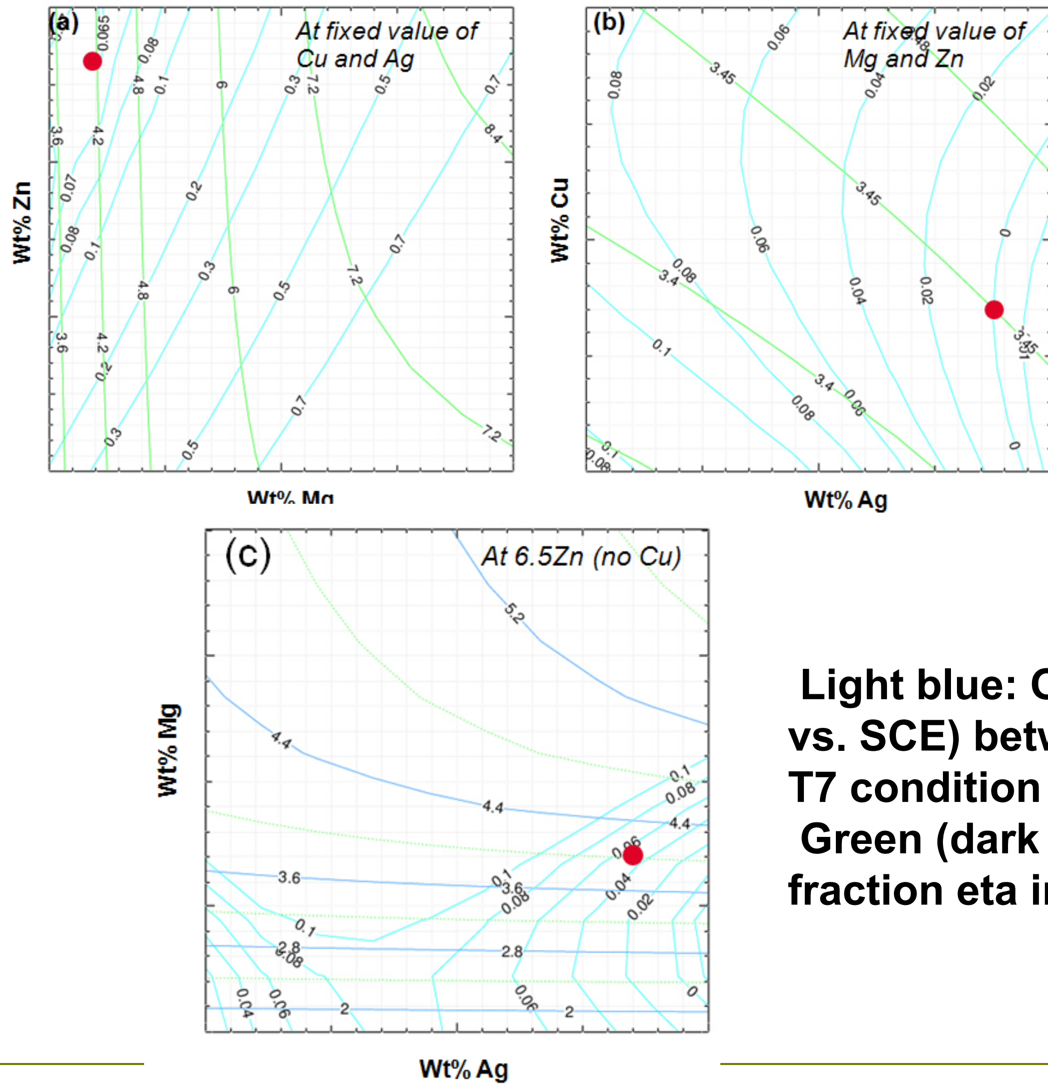


Electrochemical difference between matrix and precipitates

Existing QuesTek models
- **Phase stability, precipitation kinetics**
- **Strength**

New alloy design

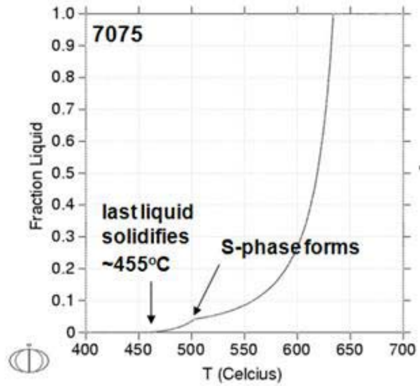
QuesTek "OCP" designs utilizing implemented models

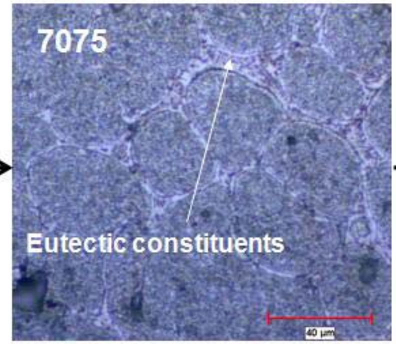


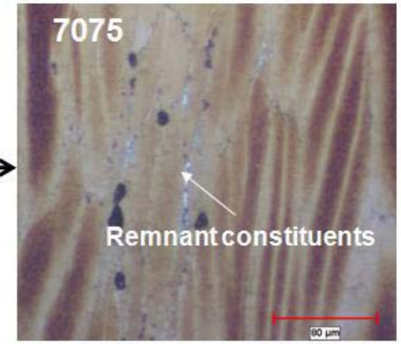
Light blue: OCP difference (in V vs. SCE) between matrix and eta in T7 condition

Green (dark blue in (c)): Phase-fraction eta in T7 condition

Simulated solidification curves and experimental micrographs for alloy 7075 and QuesTek alloy Al-1B





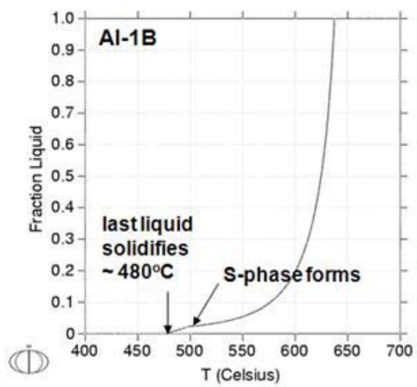


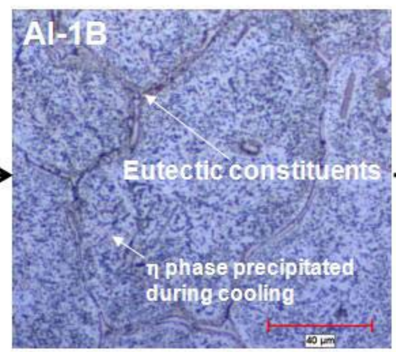
Solidification simulations for 7075 and QuesTek Al-1B alloy

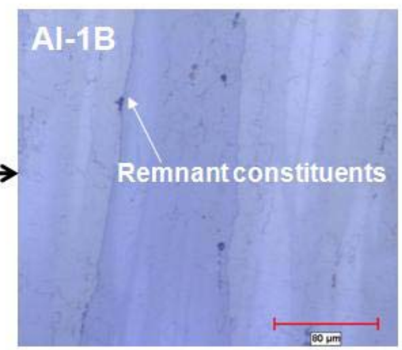
As-cast + stress-relieved microstructure

Homogenized + T73 heat-treated microstructure

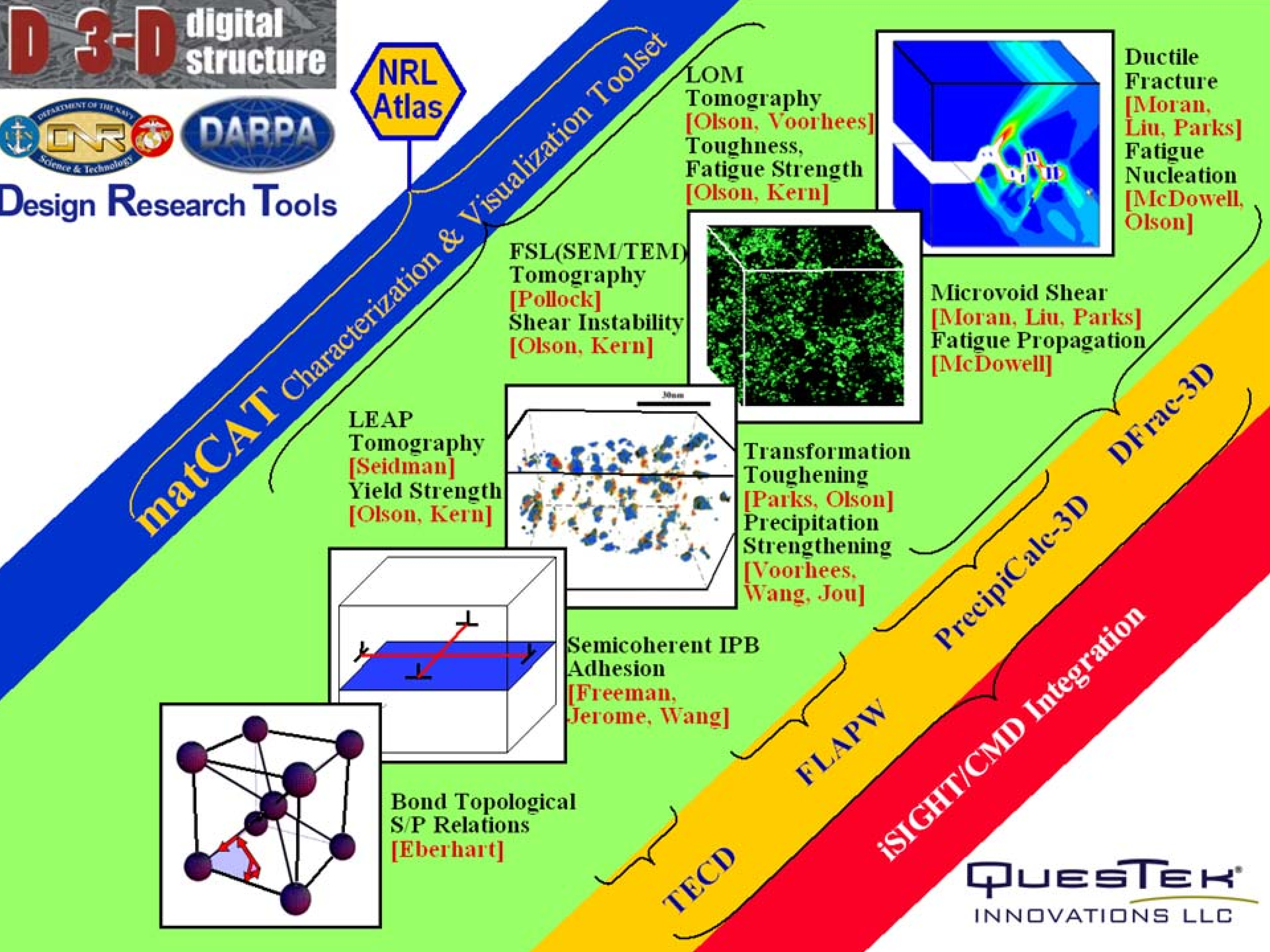
White: Undissolved S-phase/eta
Black: Al_7Cu_2Fe







Fully dissolve soluble solidification constituents by selecting optimal solidification behavior and optimal homogenization treatment

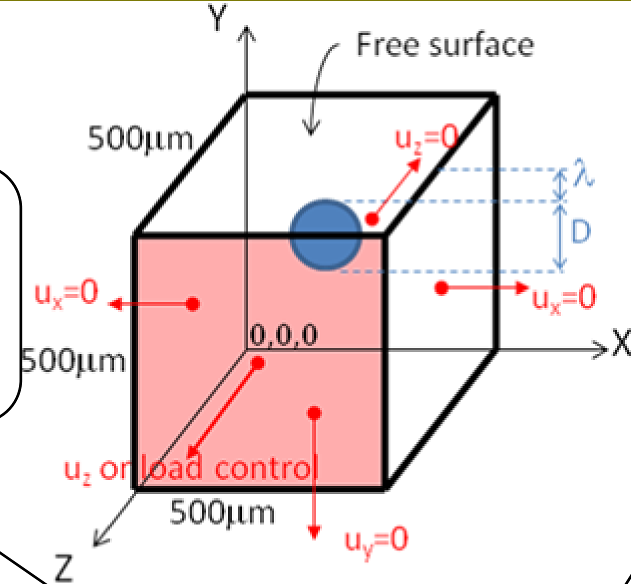


D 3-D digital structure
DARPA
Design Research Tools
NRL Atlas
matCAT Characterization & Visualization Toolset
LOM Tomography
[Olson, Voorhees]
Toughness, Fatigue Strength
[Olson, Kern]
Ductile Fracture
[Moran, Liu, Parks]
Fatigue Nucleation
[McDowell, Olson]
FSL(SEM/TEM) Tomography
[Pollock]
Shear Instability
[Olson, Kern]
Microvoid Shear
[Moran, Liu, Parks]
Fatigue Propagation
[McDowell]
30nm
LEAP Tomography
[Seidman]
Yield Strength
[Olson, Kern]
Transformation Toughening
[Parks, Olson]
Precipitation Strengthening
[Voorhees, Wang, Jou]
Semicoherent IPB Adhesion
[Freeman, Jerome, Wang]
Bond Topological S/P Relations
[Eberhart]
DFrac-3D
PrecipiCalc-3D
FLAPW
TECD
iSIGHT/CMD Integration
QuesTek INNOVATIONS LLC

MSC Fatigue Modeling Approach

Input to Microstructure-Sensitive Fatigue Life Prediction

FEM Model:
- $(500\mu m)^3$ box
- one embedded anomaly
- one free surface
- loading or displacement control along z-axis

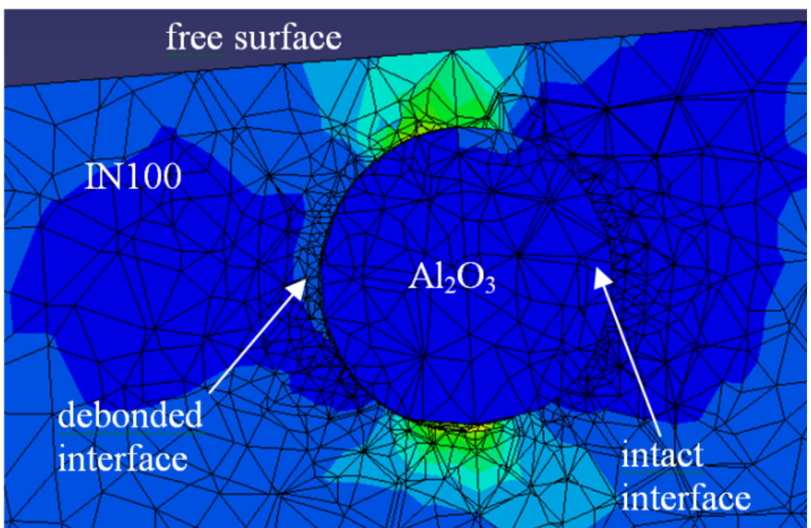


Test Conditions (from *):
- σ=1100 or 1200MPa
- T=650°C
- R=0.05

Microstructure:
- partially debonded NMP (Al_2O_3), intact NMP (Al_2O_3), or pore; distances to free surface, size extremes (from *)
- mesh — grain size, orientation

IN100 crystal plasticity UMAT developed by GIT under DARPA AIM

ABAQUS cyclic loading simulations

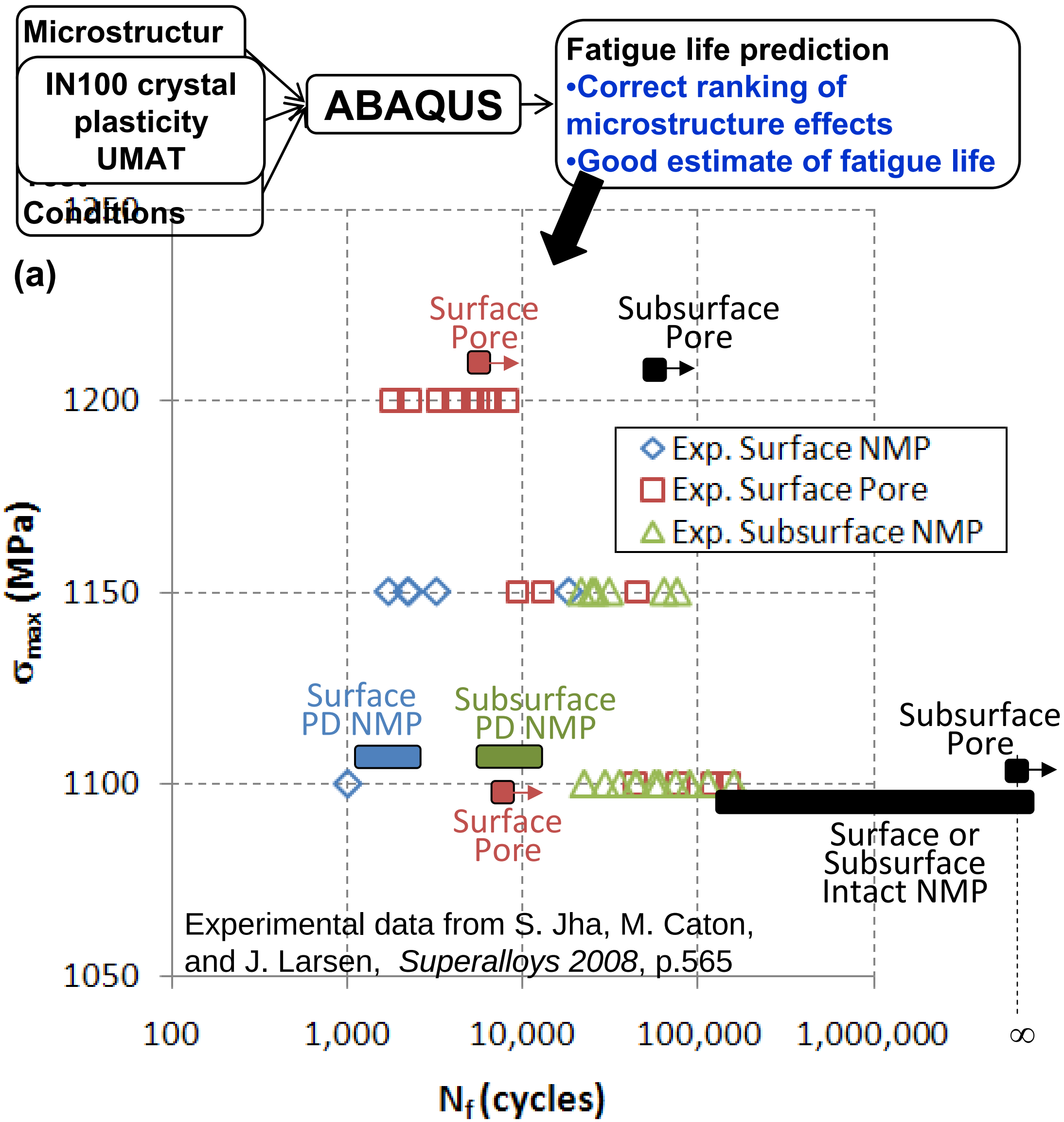


* S. Jha, M. Caton, and J. Larsen, *Superalloys 2008*, p.565

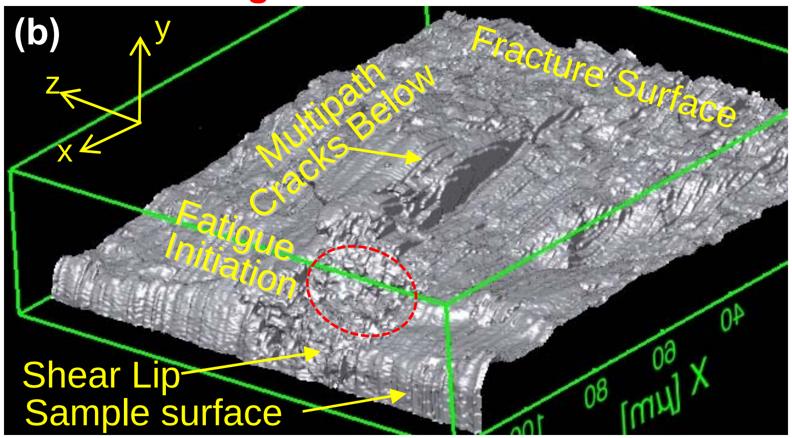
Fatigue Modeling Accomplishments

QuesTek Innovations LLC · Georgia Tech · Rolls-Royce

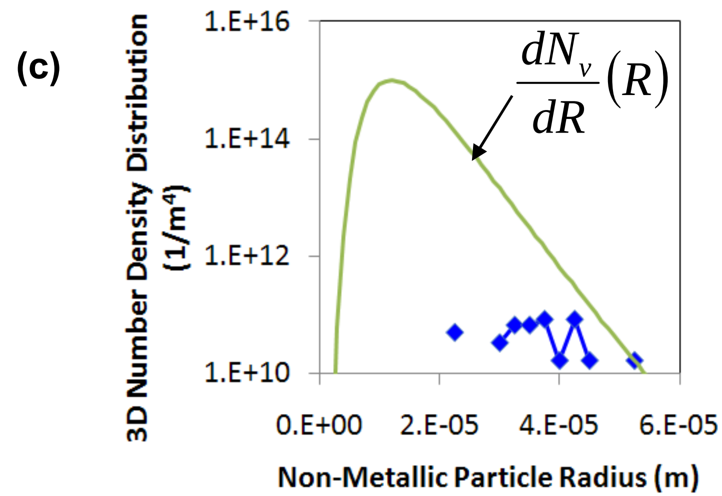
- **Demonstrated feasibility of microstructure-sensitive fatigue simulation and fatigue life prediction**



- **3D Tomographic Reconstruction Illustrated Microstructure Features Around Fatigue Initiation Site**



- **Synthesized fractographic and metallograhic data for NMP/pores**

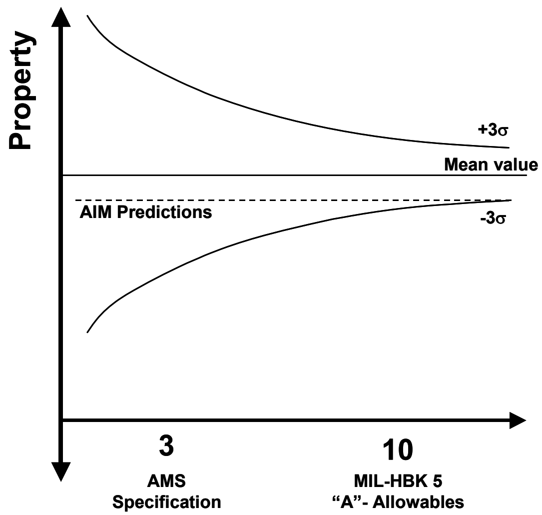


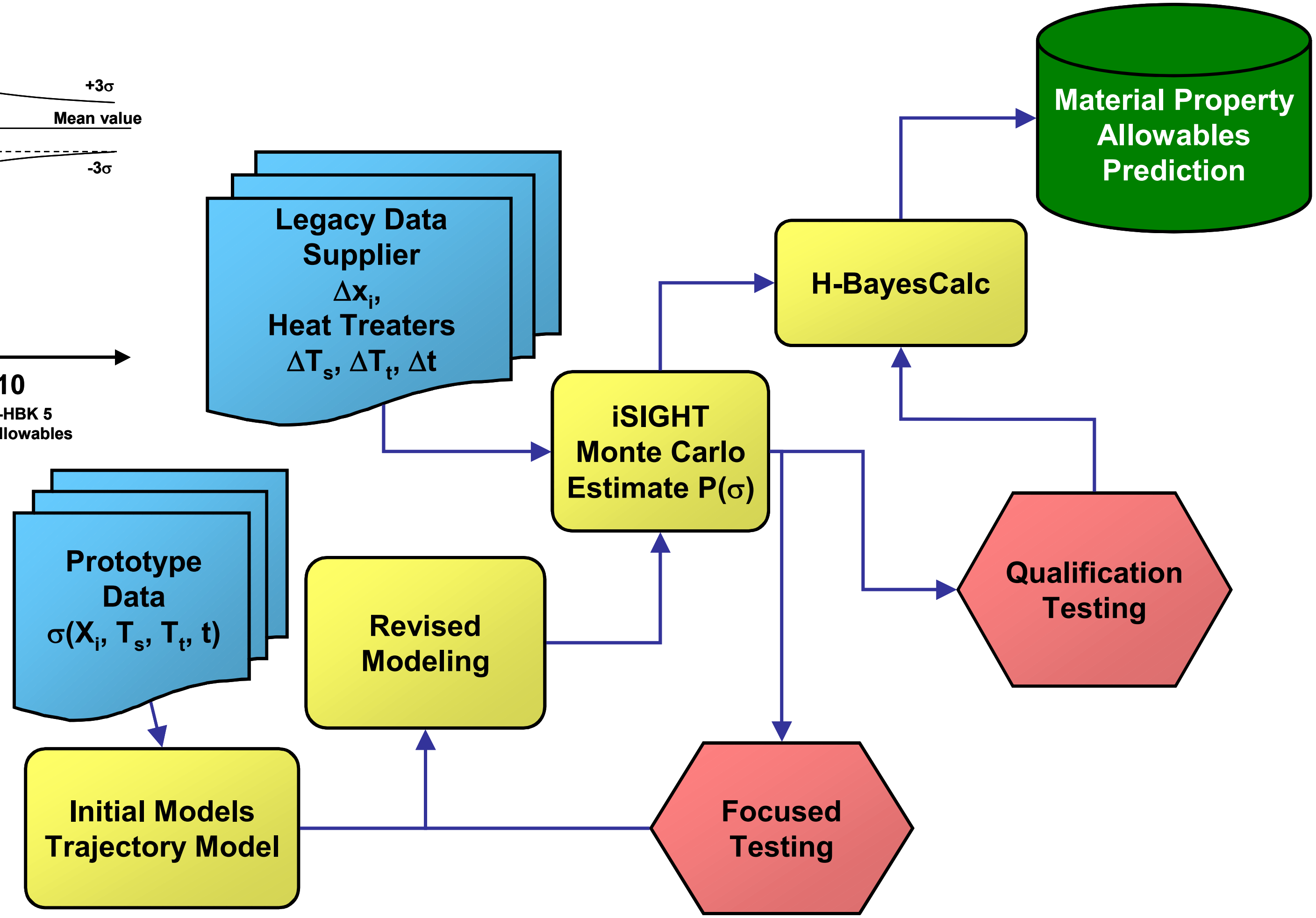
- **Developed approaches to incorporate dwell effects in transition zone**

Material Qualification

- SAE – Aerospace Materials Specification (AMS)
  - This is the material procurement document
  - Data: 3 heats, 30 tensile, 30 fracture toughness
    - Analysis/approval by Battelle Memorial
  - Document: draft an AMS document
    - Approval by AMS subcommittee
    - Approval by AMS – Aerospace Council
- Metallic Material Properties Development and Standardization (MMPDS)
  - This is the design allowables document
  - Data: 10 heats, 100 tensile, 30 fracture toughness, 20 compression, 20 shear, 20 pin bearing (e/D = 1.5, 2.0), physical properties, etc..
    - Analysis by Battelle Memorial
    - Approval by MMPDS committee and FAA

Accelerating the Qualification Cycle

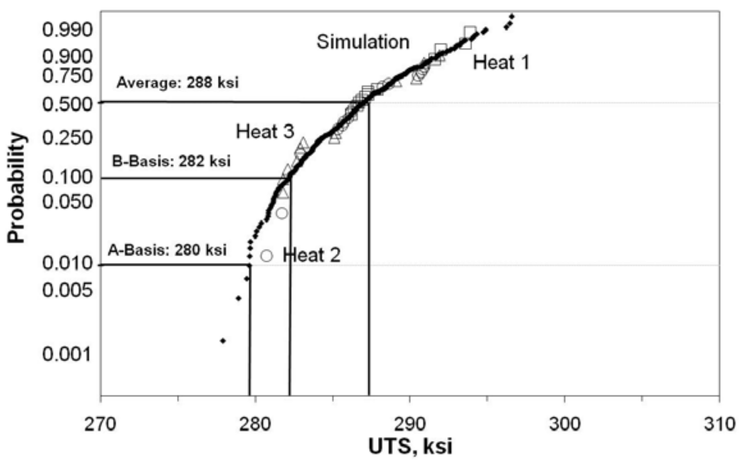




AIM Application Example: Ferrium S53®

Data generated for 3 melts/Simulations for 10

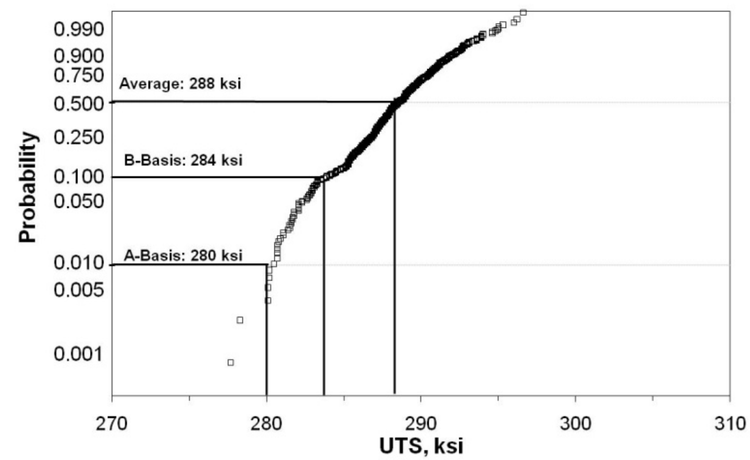
- **Predicted A-basis minimum = 280 ksi UTS**



Full Data Development →

Data generation for 10 melts

- **A-basis minimum: 280 ksi UTS**



- AIM has demonstrated reliable predictions for design minimums
- Allows designers to consider alloys prior to full design allowable development
- Reduce costs and risks for material design and development

Flying Cybersteels

- S53 Field service evaluation (approved August, 2010)
  - 6 to 24 months in test to determine preventative maintenance cycles

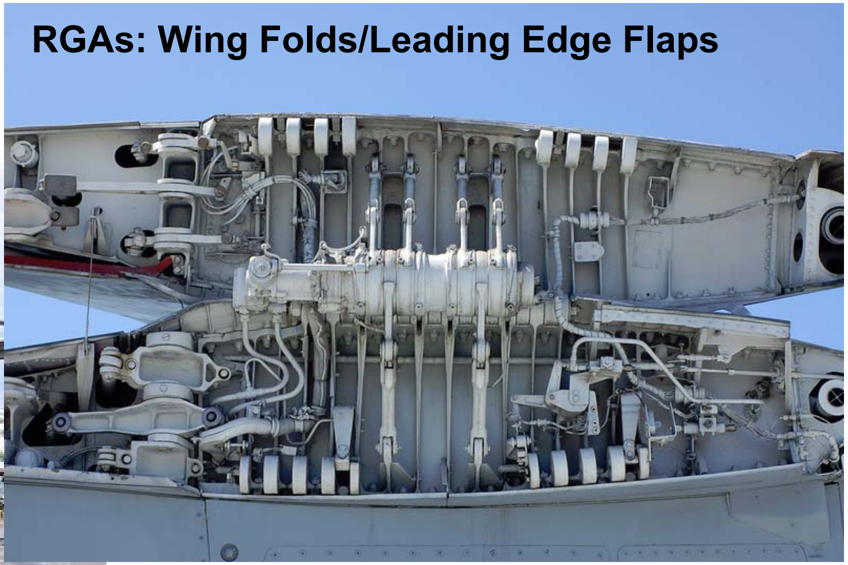
Experience lets us expand to new platforms …

Original Demonstrations

New Platforms

… and to new applications

Capability extensions such as new surface hardening processes allow us to explore applications where life is limited by wear…



The next frontier…

hydrogen 1 H 1.0079																		helium 2 He 4.0026
lithium 3 Li 6.941	beryllium 4 Be 9.0122												boron 5 B 10.811	carbon 6 C 12.011	nitrogen 7 N 14.007	oxygen 8 O 15.999	fluorine 9 F 18.998	neon 10 Ne 20.180
sodium 11 Na 22.990	magnesium 12 Mg 24.305												aluminium 13 Al 26.982	silicon 14 Si 28.086	phosphorus 15 P 30.974	sulfur 16 S 32.065	chlorine 17 Cl 35.453	argon 18 Ar 39.948
potassium 19 K 39.098	calcium 20 Ca 40.078		scandium 21 Sc 44.956	titanium 22 Ti 47.867	vanadium 23 V 50.942	chromium 24 Cr 51.996	manganese 25 Mn 54.938	iron 26 Fe 55.845	cobalt 27 Co 58.933	nickel 28 Ni 58.693	copper 29 Cu 63.546	zinc 30 Zn 65.39	gallium 31 Ga 69.723	germanium 32 Ge 72.61	arsenic 33 As 74.922	selenium 34 Se 78.96	bromine 35 Br 79.904	krypton 36 Kr 83.80
rubidium 37 Rb 85.468	strontium 38 Sr 87.62		yttrium 39 Y 88.906	zirconium 40 Zr 91.224	niobium 41 Nb 92.906	molybdenum 42 Mo 95.94	technetium 43 Tc [98]	ruthenium 44 Ru 101.07	rhodium 45 Rh 102.91	palladium 46 Pd 106.42	silver 47 Ag 107.87	cadmium 48 Cd 112.41	indium 49 In 114.82	tin 50 Sn 118.71	antimony 51 Sb 121.76	tellurium 52 Te 127.60	iodine 53 I 126.90	xenon 54 Xe 131.29
caesium 55 Cs 132.91	barium 56 Ba 137.33	57-70 *	lutetium 71 Lu 174.97	hafnium 72 Hf 178.49	tantalum 73 Ta 180.95	tungsten 74 W 183.84	rhenium 75 Re 186.21	osmium 76 Os 190.23	iridium 77 Ir 192.22	platinum 78 Pt 195.08	gold 79 Au 196.97	mercury 80 Hg 200.59	thallium 81 Tl 204.38	lead 82 Pb 207.2	bismuth 83 Bi 208.98	polonium 84 Po [209]	astatine 85 At [210]	radon 86 Rn [222]
francium 87 Fr [223]	radium 88 Ra [226]	89-102 * *	lawrencium 103 Lr [262]	rutherfordium 104 Rf [261]	dubnium 105 Db [262]	seaborgium 106 Sg [266]	bohrium 107 Bh [264]	hassium 108 Hs [269]	meitnerium 109 Mt [268]	ununnilium 110 Uun [271]	unununium 111 Uuu [272]	ununbium 112 Uub [277]		ununquadium 114 Uuq [289]				

* Lanthanide series	lanthanum 57 La 138.91	cerium 58 Ce 140.12	praseodymium 59 Pr 140.91	neodymium 60 Nd 144.24	promethium 61 Pm [145]	samarium 62 Sm 150.36	europium 63 Eu 151.96	gadolinium 64 Gd 157.25	terbium 65 Tb 158.93	dysprosium 66 Dy 162.50	holmium 67 Ho 164.93	erbium 68 Er 167.26	thulium 69 Tm 168.93	ytterbium 70 Yb 173.04
* * Actinide series	actinium 89 Ac [227]	thorium 90 Th 232.04	protactinium 91 Pa 231.04	uranium 92 U 238.03	neptunium 93 Np [237]	plutonium 94 Pu [244]	americium 95 Am [243]	curium 96 Cm [247]	berkelium 97 Bk [247]	californium 98 Cf [251]	einsteinium 99 Es [252]	fermium 100 Fm [257]	mendelevium 101 Md [258]	nobelium 102 No [259]

Using ICME to Significantly Improve Equipment Performance, Affordability and EHS

Marine Corps: M67854-05-C-0025

Army : W15QKN-09-C-0026

Navy: N65538-09-M-0088

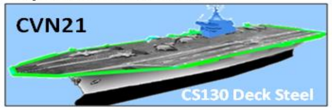
NAVAIR: N68335-07-C-0302
and N68335-08-C-0288

ONR: N00014-05-M-0250
NAVAIR: N68335-06-C-0339

DoD/ESTCP; Air Force, Ogden UT; General Atomics

Army/Picatinny:
DAAE30-01-9-0800

Navy/ONR: N00014-05-C-0241



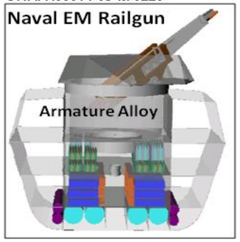
Army/Picatinny:
W15QKN-05-P-0181

ONR: N00014-07-M-0445 STTR-I

Army W911W6-09-C-0001

AFRL FA9550-09-C-0027

ONR: N00014-09-M-0220



ONR: N00014-08-M-0309

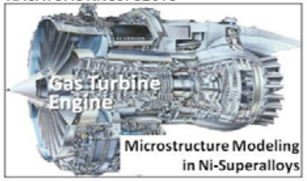
Marine Corps: M67854-10-C-6502

NAVAIR: N68335-09-C-0215

NAVAIR: N68335-07-C-0428

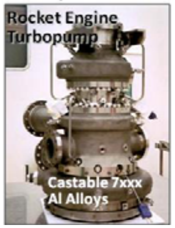
NAVAIR: N68335-05-C-0207 and
N68335-07-C-0108

NASA /GRC NNC07CB01C

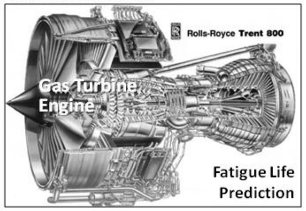


AFRL/Pratt & Whitney
Rocketdyne PO 4410000226

AFRL/Pratt & Whitney
Rocketdyne NR07461741



AFRL FA8650-09-M-5216



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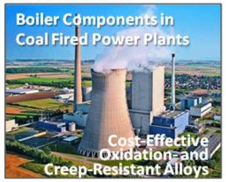
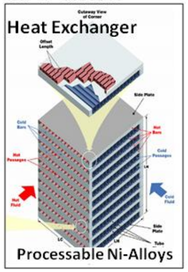


NSF IIP-0839678



DOE: DE-SC0002475

Thank You

Questions?

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